

10/665, 314

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NEWS 6 JUL 16 CAplus enhanced with French and German abstracts
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NEWS 11 AUG 06 BEILSTEIN updated with new compounds
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NEWS 14 AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 15 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
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NEWS 17 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 18 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 19 SEP 13 FORIS renamed to SOFIS
NEWS 20 SEP 13 INPADOCDB enhanced with monthly SDI frequency
NEWS 21 SEP 17 CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 22 SEP 17 CAplus coverage extended to include traditional medicine patents
NEWS 23 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 24 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

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COST IN U.S. DOLLARS

FULL ESTIMATED COST

| SINCE FILE
ENTRY | TOTAL
SESSION |
|---------------------|------------------|
| 0.21 | 0.21 |

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DICTIONARY FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4

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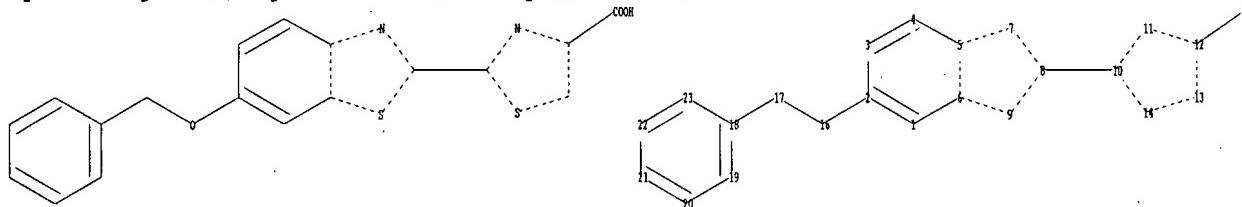
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ring bonds :
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18-19 18-23 19-20 20-21 21-22 22-23

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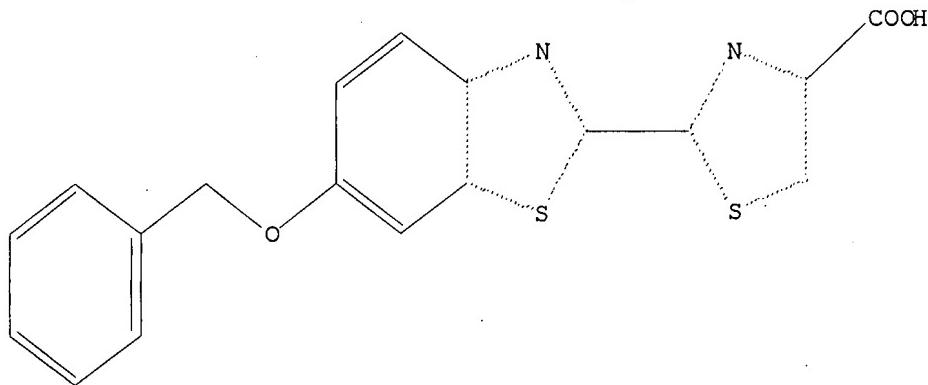
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20:Atom 21:Atom 22:Atom 23:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

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SAMPLE SCREEN SEARCH COMPLETED - 189 TO ITERATE

100.0% PROCESSED 189 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 full

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100.0% PROCESSED 4492 ITERATIONS
SEARCH TIME: 00.00.01

11 ANSWERS

L3 11 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

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=> s 13
L4          2 L3

=> d ibib abs hitstr tot
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ACCESSION NUMBER: 20061279865 CAPLUS

DOCUMENT NUMBER: 146:57589

TITLE: Luminogenic and fluorogenic compounds and methods to detect molecules or conditions

INVENTOR(S): Daily, William; Hawkins, Erik; Klaubert, Dieter; Liu, Jianquen; Heizenheimer, Poncho; Scurria, Michael; Shultz, John W.; Unch, James; Wood, Keith V.; Zhou, Weihui Valley, Michael P.; Cali, James J.

PATENT ASSIGNEE(S): Promega Corporation, USA

SOURCE: PCT Int. Appl., 328pp.

CODEN: PIXKD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2006130551 | A2 | 20061207 | WO 2006-US20731 | 20060530 |
| WO 2006130551 | A8 | 20070201 | | |
| WO 2006130551 | A3 | 20070503 | | |
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| RU: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CL, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA | | | | |
| US 2007015790 | A1 | 20070118 | US 2006-444145 | 20060531 |
| PRIORITY APPN. INFO.: | | | US 2005-685957P | P 20050531 |
| | | | US 2005-693034P | P 20050621 |
| | | | US 2005-692925P | P 20050622 |
| | | | US 2006-79045P | P 20060407 |

OTHER SOURCE(S): MARPAT 146:57589

AB A method to detect the presence or amount of at least one mol. in a sample which employs a derivative of luciferin or a derivative of a fluorophore is provided.

IT 916661-52-4 916661-53-5 916661-59-1

916661-63-7

RL: BUV (Biological use, unclassified); BIOL (Biological study); USES (Uses) (luminogenic and fluorogenic compds. and methods to detect mols. or conditions)

RN 916661-52-4 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-[(2,3,4,5,6-pentafluorophenyl)methoxy]-2-benzothiazolyl]-, (4S)- (CA INDEX NAME)

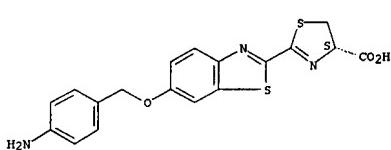
Absolute stereochemistry.

(Continued)

RN 916661-63-7 CAPLUS

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Absolute stereochemistry.



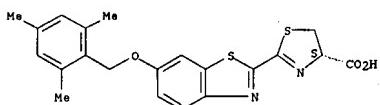
IT 916660-57-6P 916661-30-8P

RL: BUV (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (luminogenic and fluorogenic compds. and methods to detect mols. or conditions)

RN 916660-57-6 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-[(2,4,6-trimethylphenyl)methoxy]-2-benzothiazolyl]-, (4S)- (CA INDEX NAME)

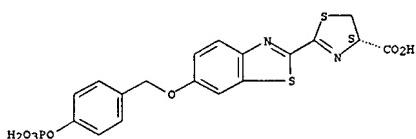
Absolute stereochemistry.



RN 916661-30-8 CAPLUS

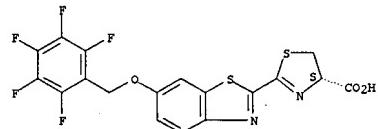
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Absolute stereochemistry.



● x NH3

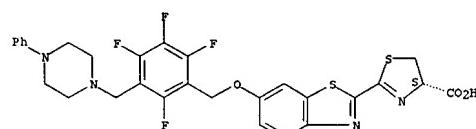
(Continued)



RN 916661-53-5 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-[(2,3,4,6-tetrafluoro-5-phenyl)methoxy]-2-benzothiazolyl]-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.

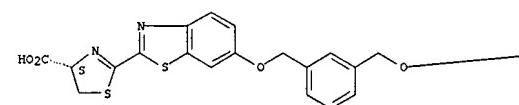


RN 916661-59-1 CAPLUS

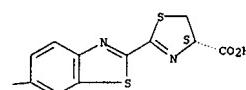
CN 4-Thiazolecarboxylic acid, 2,2'-(1,3-phenylenebis(methyleneoxy-6,2-benzothiazolediy))bis[4,5-dihydro-, (4S,4'S)- (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



(Continued)

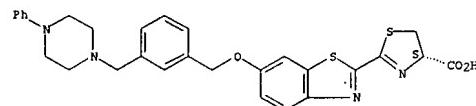
IT 916660-53-2P 916660-55-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (luminogenic and fluorogenic compds. and methods to detect mols. or conditions)

RN 916660-53-2 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-[(3-[(4-phenyl-1-piperazinyl)methyl]phenyl)methoxy]-2-benzothiazolyl]-, (4S)- (CA INDEX NAME)

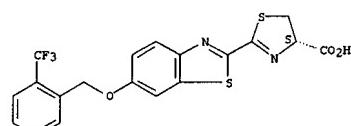
Absolute stereochemistry.



RN 916660-55-4 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-[(2-(trifluoromethyl)phenyl)methoxy]-2-benzothiazolyl]-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004270174 CAPLUS

DOCUMENT NUMBER: 140299425

TITLE: Luminescent cytochrome P 450 assay using luciferase, luciferin derivatives and pyrophosphatase, and drug screening applications

INVENTOR(S): Cali, James J.; Klaubert, Dieter; Daily, William; Ho, Samuel Kin Sang; Frackman, Susan; Hawkins, Erika; Wood, Keith V.

PATENT ASSIGNEE(S): Promega Corporation, USA

SOURCE: PCT Int. Appl., 130 pp.

CODEN: PIXKD2

DOCUMENT TYPE:

Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
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| WO 2004027378 | A2 | 20040401 | WO 2003-US29078 | 20030916 |
| WO 2004027378 | A3 | 20041125 | | |
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| CA 2497560 | A1 | 20040408 | AU 2003267245 | 20030916 |
| AU 2003267245 | B2 | 20070712 | AU 2003267245 | |
| EP 1546162 | A2 | 20050629 | EP 2003-749715 | 20030916 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | A1 | 20040408 | AU 2004171099 | 20030919 |
| JP 2006508339 | T | 20060309 | JP 2004-537859 | 20030916 |
| US 2004171099 | A1 | 20040902 | US 2003-665314 | 20030919 |
| | | | US 2002-4122545 | P 20020920 |
| | | | US 2003-483309P | P 20030627 |
| PRIORITY APILN. INFO.: | | | WO 2003-US29078 | W 20030916 |

OTHER SOURCE(S): MARPAT 140:299425

AB The present invention provides methods, compns., substrates, and kits useful for analyzing the metabolic activity in cells, tissue, and animals and for screening test compds. for their effect on cytochrome P 450 activity. In particular, a one-step and two-step methods using luminescent mol., e.g., luciferin or coelenterazines, that are cytochrome P 450 substrates and that are also bioluminescent enzyme, e.g., luciferase, pro-substrates are provided. Upon addition of the luciferin derivative or other luminescent mol. into a P 450 reaction, the P 450 enzyme metabolizes the mol. into a bioluminescent enzyme substrate, e.g., luciferin and/or luciferin derivative metabolite, in a P 450 reaction. The resulting metabolite(s) serves as a substrate of the bioluminescent enzyme, e.g., luciferase, a second light-generating reaction. Luminescent cytochrome P 450 assays with low background signals and high sensitivity are disclosed and isomeric selectivity is demonstrated. The present invention also provides an improved method for performing luciferase reactions which employs added pyrophosphatase to remove inorg. pyrophosphate, a luciferase inhibitor which may be present in the reaction mixture as a contaminant or may be generated during the reaction. The

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
present method further provides a method for stabilizing and prolonging the luminescent signal in a luciferase-based assay using luciferase stabilizing agents such as reversible luciferase inhibitors.

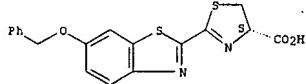
IT 676460-32-6P 676460-33-6P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses); (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

RN 676460-32-5 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-2-[6-(phenylmethoxy)-2-benzothiazolyl]-, (4S)- (CA INDEX NAME)

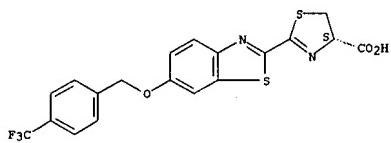
Absolute stereochemistry.



RN 676460-33-6 CAPLUS

CN 4-(trifluoromethyl)phenylmethoxy-2-benzothiazolyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



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COST IN U.S. DOLLARS
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          ENTRY        SESSION
FULL ESTIMATED COST           11.01     183.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE             -1.56      -1.56
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 DICTIONARY FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4

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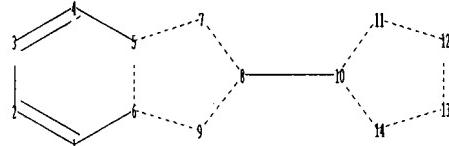
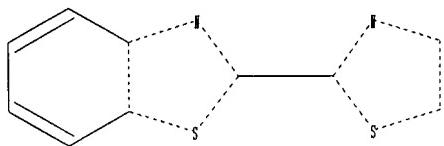
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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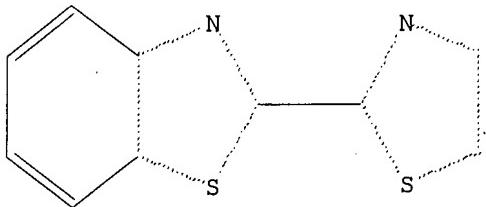


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11:Atom 12:Atom 13:Atom 14:Atom
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L5 STRUCTURE UPLOADED

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L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 376 TO 1104

L6 37 SEA SSS SAM L5

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L7 600 SEA SSS FUL L5

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ENTRY SESSION
CA SUBSCRIBER PRICE 0.00 -1.56

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FILE LAST UPDATED: 4 Oct 2007 (20071004/ED)

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=> s 17
L8 1155 L7

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FULL ESTIMATED COST 2.35 357.77

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
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CA SUBSCRIBER PRICE 0.00 -1.56

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DICTIONARY FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4

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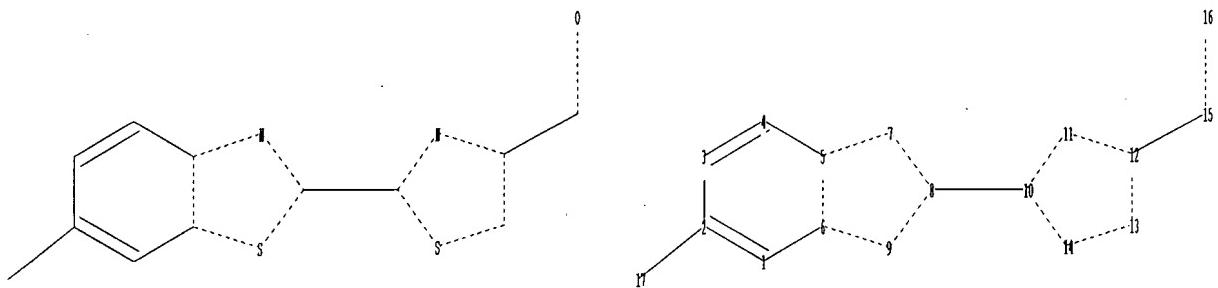
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10665314b.str



chain nodes :

15 16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

2-17 8-10 12-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

15-16

exact bonds :

2-17 8-10 12-15

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

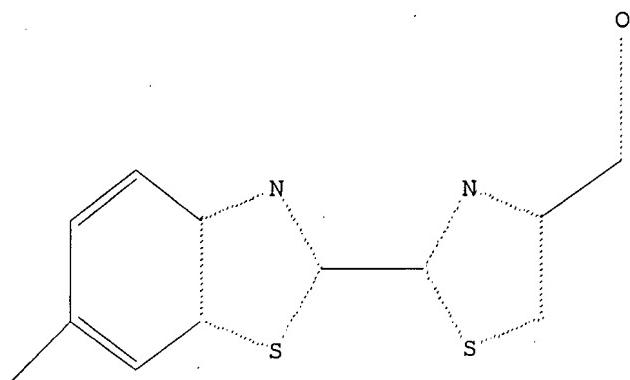
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS

L9 STRUCTURE UPLOADED

=> d

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19

SAMPLE SEARCH INITIATED 13:00:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=> s 19 full
FULL SEARCH INITIATED 13:00:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 58 TO ITERATE

100.0% PROCESSED 58 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L11 2 SEA SSS FUL L9

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
SESSION
FULL ESTIMATED COST ENTRY 172.10 529.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
SESSION
CA SUBSCRIBER PRICE ENTRY 0.00 -1.56

FILE 'CAPLUS' ENTERED AT 13:00:45 ON 05 OCT 2007
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FILE COVERS 1907 - 5 Oct 2007 VOL 147 ISS 16
FILE LAST UPDATED: 4 Oct 2007 (20071004/ED)

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<http://www.cas.org/infopolicy.html>

=> s 111

L12 1 L11

| | | |
|--|------------------|---------------|
| => fil reg | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 0.47 | 530.34 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.56 |

FILE 'REGISTRY' ENTERED AT 13:01:11 ON 05 OCT 2007
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STRUCTURE FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4
DICTIONARY FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

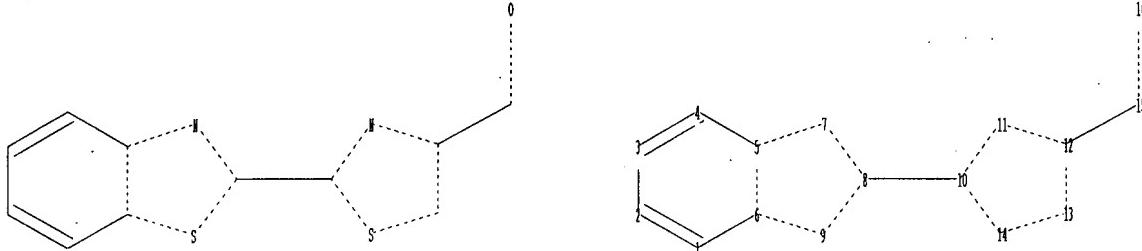
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10665314c.str



chain nodes :

15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

8-10 12-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

exact/norm bonds :

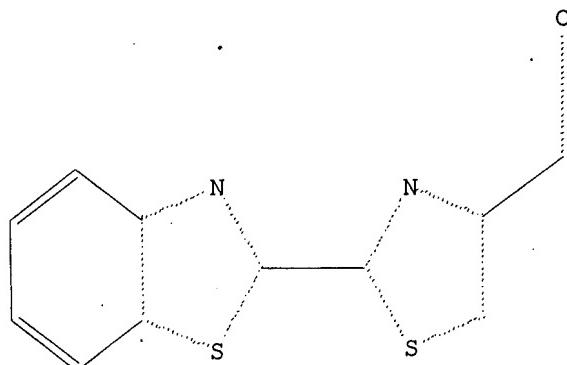
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14
15-16
exact bonds :
8-10 12-15

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS

L13 STRUCTURE UPLOADED

=> d

L13 HAS NO ANSWERS
L13 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 13:01:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS 21 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 173 TO 747
PROJECTED ANSWERS: 146 TO 694

L14 21 SEA SSS SAM L13

=> s l13 full
FULL SEARCH INITIATED 13:01:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 388 TO ITERATE

100.0% PROCESSED 388 ITERATIONS 320 ANSWERS
SEARCH TIME: 00.00.01

L15 320 SEA SSS FUL L13

| | | | |
|--|------------------|---------------|--|
| => fil caplus | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 172.10 | 702.44 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -1.56 | |

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 FILE LAST UPDATED: 4 Oct 2007 (20071004/ED)

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| | | | |
|--|------------------|---------------|--|
| => s 115 | | | |
| L16 920 L15 | | | |
| => fil reg | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 0.47 | 702.91 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -1.56 | |

FILE 'REGISTRY' ENTERED AT 13:02:30 ON 05 OCT 2007
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 DICTIONARY FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

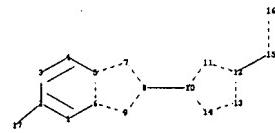
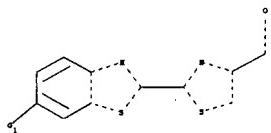
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10665314d.str



chain nodes :

15 16 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

2-17 8-10 12-15 15-16

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-6 2-3 2-17 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13

13-14 15-16

exact bonds :

8-10 12-15

G1:Cb,Cy,Hy,Ak

Match level :

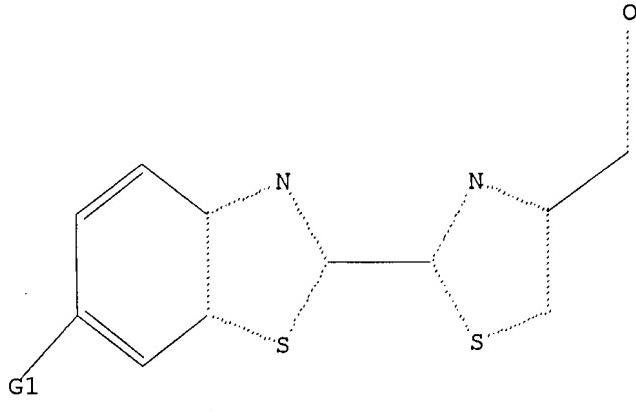
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS

L17 STRUCTURE UPLOADED

=> d

L17 HAS NO ANSWERS
L17 STR



G1 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 117

SAMPLE SEARCH INITIATED 13:02:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 173 TO 747
PROJECTED ANSWERS: 0 TO 0

L18 0 SEA SSS SAM L17

=> s 117 full
FULL SEARCH INITIATED 13:02:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 388 TO ITERATE

100.0% PROCESSED 388 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L19 4 SEA SSS FUL L17

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
CA SUBSCRIBER PRICE ENTRY SESSION

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 172.10 | 875.01 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.56 |

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FILE LAST UPDATED: 4 Oct 2007 (20071004/ED)

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=> s 119

L20 3 L19

=> d ibib abs hitstr tot

ACCESSION NUMBER: 2004:722833 CAPLUS

DOCUMENT NUMBER: 141:217988

TITLE: Signalling compounds for use in methods of detecting

hydrogen peroxide

INVENTOR(S): Akhavan-Tafti, Hashem; Eickholt, Robert A.; Lauwers,

Kenneth S.; Handley, Richard S.

PATENT ASSIGNEE(S): Lumigen, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 33 pp., Cont.-in-part of U.S.

Ser. No. 371,053.

CODEN: USXKCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| US 2004171098 | A1 | 20040902 | US 2003-600928 | 20030620 |
| US 6919463 | B2 | 20050719 | | |
| US 2004166539 | A1 | 20040826 | US 2003-371053 | 20030220 |
| WO 2004074810 | A2 | 20040902 | WO 2004-US2020 | 20040217 |
| WO 2004074810 | A3 | 20050825 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1594855 | A2 | 20051116 | EP 2004-711799 | 20040217 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | T | 20060907 | JP 2006-502994 | 20040217 |
| JP 2006520465 | | | US 2003-371053 | 20030220 |
| PRIORITY APPLN. INFO.: | | | US 2003-600928 | A 20030620 |
| | | | WO 2004-US2020 | W 20040217 |

OTHER SOURCE(S): MARPAT 141:217988

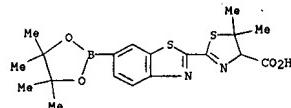
AB Compds. useful for detecting a source of hydrogen peroxide are disclosed wherein a signalling compound of the formula: Sig-B-(OR)_2 (OR_2 is a boron atom and R and R₂ are independently selected from hydrogen and lower alkyl groups) and can be joined together as a straight or branched alkylene chain forming a five or six membered ring. A detectable product compound Sig-OH is produced and detected by measuring color, fluorescence, chemiluminescence, or bioluminescence. The signalling compound itself does not possess the detectable property or does so only to a very weak degree. The compds. can be used for detection in assays for peroxide or peroxide-producing enzymes and in assays employing enzyme-labeled specific binding pairs.

IT 741253-14-5P 741253-17-8P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (methods and compds. for detection of hydrogen peroxide)

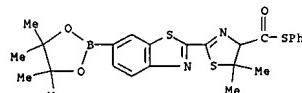
RN 741253-14-5 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-5,5-dimethyl-2-[6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-benzothiazolyl]-, S-phenyl ester (CA INDEX NAME)



RN 741253-17-8 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-5,5-dimethyl-2-[6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-benzothiazolyl]-, S-phenyl ester (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:701711 CAPLUS

DOCUMENT NUMBER: 141:217987

TITLE: Signalling compounds and methods for detecting hydrogen peroxide

INVENTOR(S): Akhavan-Tafti, Hashem; Eickholt, Robert A.; Lauwers, Kenneth S.; Handley, Richard S.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 32 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| US 2004166539 | A1 | 20040826 | US 2003-371053 | 20030220 |
| US 2004171098 | A1 | 20040902 | US 2003-600928 | 20030620 |
| US 6919463 | B2 | 20050719 | | |
| WO 2004074810 | A2 | 20040902 | WO 2004-US2020 | 20040217 |
| WO 2004074810 | A3 | 20050825 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1594855 | A2 | 20051116 | EP 2004-711799 | 20040217 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | T | 20060907 | JP 2006-502994 | 20040217 |
| JP 2006520465 | | | US 2003-371053 | 20030220 |
| PRIORITY APPLN. INFO.: | | | US 2003-600928 | A 20030620 |
| | | | WO 2004-US2020 | W 20040217 |

OTHER SOURCE(S): MARPAT 141:217987

AB Methods and compound useful for detecting a source of hydrogen peroxide are disclosed wherein a signalling compound of the formula: Sig-B-(OR)_2 (OR_2 is a boron atom and R and R₂ are independently selected from hydrogen and lower alkyl groups) and can be joined together as a straight or branched alkylene chain forming a ring or as an aromatic ring. A detectable product compound

Sig-OH

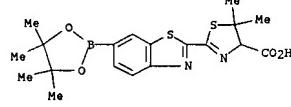
Sig-OH - is produced and detected by measuring color, absorbance, fluorescence, chemiluminescence, or bioluminescence. The signalling compound itself does not possess the detectable property or does so only to a very weak degree. The methods can be used as a detectable signal in assays for peroxide or peroxide-producing enzymes and in assays employing enzyme-labeled specific binding pairs.

IT 741253-14-5P 741253-17-8P

RL: ARG (Analytical reagent use); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses) (methods and compds. for detection of hydrogen peroxide)

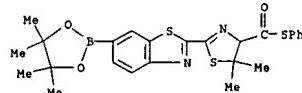
RN 741253-14-5 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-5,5-dimethyl-2-[6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-benzothiazolyl]-, S-phenyl ester (CA INDEX NAME)



RN 741253-17-8 CAPLUS

CN 4-Thiazolecarboxylic acid, 4,5-dihydro-5,5-dimethyl-2-[6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-2-benzothiazolyl]-, S-phenyl ester (CA INDEX NAME)



L20 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS ON STN

ACCESSION NUMBER: 1970:18740 CAPLUS

DOCUMENT NUMBER: 72:18740

TITLE: Substrate-binding properties of firefly luciferase.

I. Luciferin-binding site

AUTHOR(S): Denburg, Jeffrey; Lee, Reiko; Takasaka, McElroy, W. D.

CORPORATE SOURCE: Johns Hopkins Univ., Baltimore, MD, USA

SOURCE: Archives of Biochemistry and Biophysics (1969),

134(2), 381-94

CODEN: ABBA4; ISSN: 0003-9861

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Various techniques were used for characterization of the luciferin-binding site of the firefly luciferase. Both equilibrium-dialysis and fluorescence-titration techniques revealed the existence of 2 identical, noninteracting binding sites for dehydroluciferin, which is a potent competitive inhibitor. Kinetically obtained dissociation consts. of various luciferin analogs and other competitive inhibitors revealed that most of the binding energies of these compds. residue in the backbone ring structure and that various substituents did not influence the binding to any significant extent. Exceptions to this are the Me group at the 6-position of the benzothiazole ring and the carboxylic acid group. The binding energy of the luciferin backbone structure to the luciferin-binding site is 7.5 kcal/mole. Two parts of the luciferin mol., the benzothiazole ring portion and the thiazoline ring portion, contribute 6.0 kcal/mole and 1.5 kcal/mole, resp., to the binding energy. Comparison of the binding energies of several heterocyclic compds. structurally related to benzothiazole suggests that the N atom of the benzothiazole ring may be important in orienting the compound to a fixed position in the luciferin-binding site. The binding studies with N-ethylmaleimide-inactivated luciferase gave further evidence that the 2 SH groups essential for the luciferase activity are located at the luciferin binding sites, most likely 1 at each binding site. Excitation spectra of luciferase-bound dehydroluciferin indicated that the phenolic group of dehydroluciferin is in unionized form on the enzyme even in a medium of high pH. This effect and a large enhancement of the blue fluorescence peak at 440 nm suggest the environment of luciferin-binding site to be quite hydrophobic, in agreement with earlier observations.

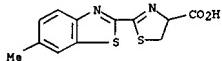
IT 23815-78-3

RL: PROC (Process)

(luciferase binding of)

RN 23815-78-3 CAPLUS

CN 2-Thiazoline-4-carboxylic acid, 2-(6-methyl-2-benzothiazolyl)- (BCI) (CA INDEX NAME)



=> log y

| | | |
|--|------------------|---------------|
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
| FULL ESTIMATED COST | 16.28 | 891.29 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | -2.34 | -3.90 |

STN INTERNATIONAL LOGOFF AT 13:03:21 ON 05 OCT 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTASEL1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * Welcome to STN International * * * * * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 JUL 02 LMEDLINE coverage updated
NEWS 3 JUL 02 SCISEARCH enhanced with complete author names
NEWS 4 JUL 02 CHEMCATS accession numbers revised
NEWS 5 JUL 02 CA/CAplus enhanced with utility model patents from China
NEWS 6 JUL 16 CAplus enhanced with French and German abstracts
NEWS 7 JUL 18 CA/CAplus patent coverage enhanced
NEWS 8 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 9 JUL 30 USGENE now available on STN
NEWS 10 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 11 AUG 06 BEILSTEIN updated with new compounds
NEWS 12 AUG 06 FSTA enhanced with new thesaurus edition
NEWS 13 AUG 13 CA/CAplus enhanced with additional kind codes for granted patents
NEWS 14 AUG 20 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 15 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 16 AUG 27 USPATOLD now available on STN
NEWS 17 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 18 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 19 SEP 13 FORIS renamed to SOFIS
NEWS 20 SEP 13 INPADOCDB enhanced with monthly SDI frequency
NEWS 21 SEP 17 CA/CAplus enhanced with printed CA page images from 1967-1998
NEWS 22 SEP 17 CAplus coverage extended to include traditional medicine patents
NEWS 23 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 24 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

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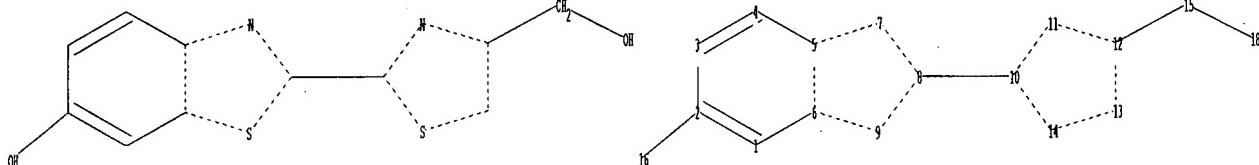
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15 16 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

2-16 8-10 12-15 15-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

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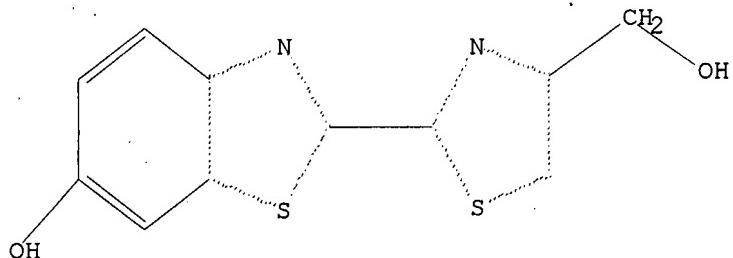
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Match level :
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11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS
L1 STR



G1 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2213 TO 3667
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 full
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FULL SCREEN SEARCH COMPLETED - 3249 TO ITERATE

100.0% PROCESSED 3249 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

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172.10 172.31

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=> s 13

L4 5 L3

=> d ibib abs hitstr tot

ACCESSION NUMBER: 2006:1279865 CAPLUS

DOCUMENT NUMBER: 146:57589

TITLE: Luminogenic and fluorogenic compounds and methods to detect molecules or conditions

INVENTOR(S): Daily, William; Hawkins, Erika; Klaubert, Dieter; Liu, Jianquani; Meisenheimer, Poncho; Scurria, Michael; Shultz, John W.; Unch, James; Wood, Keith V.; Zhou, Wenhui; Valley, Michael P.; Cali, James J.

PATENT ASSIGNEE(S): Promega Corporation, USA

SOURCE: PCT Int. Appl., 328pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2006130551 | A2 | 20061207 | WO 2006-US20731 | 20060530 |
| WO 2006130551 | A8 | 20070201 | | |
| WO 2006130551 | A3 | 20070503 | | |
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| US 2007015790 | A1 | 20070118 | US 2006-444145 | 20060531 |
| PRIORITY APPLN. INFO.: | | | US 2005-685957B | P 20050531 |
| | | | US 2005-693034P | P 20050621 |
| | | | US 2005-692925P | P 20050622 |
| | | | US 2006-79045P | P 20060407 |

OTHER SOURCE(S): MARPAT 146:57589

AB A method to detect the presence or amount of at least one mol. in a sample which employs a derivative of luciferin or a derivative of a fluorophore is provided.

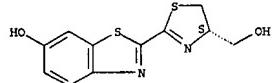
IT 676460-20-1

RL: BSU (Biological study, unclassified); BIOL (Biological study) (luminogenic and fluorogenic compds. and methods to detect mol. or conditions)

RN 676460-20-1 CAPLUS

CN 6-Benzothiazolol, 2-[{(4S)-4,5-dihydro-4-(hydroxymethyl)-2-thiazolyl}- (CA INDEX NAME)

Absolute stereochemistry.



ACCESSION NUMBER: 2004:270174 CAPLUS

DOCUMENT NUMBER: 140:299425

TITLE: Luminescent cytochrome P 450 assay using luciferase, luciferin derivatives and pyrophosphatase, and drug screening applications

INVENTOR(S): Cali, James J.; Klaubert, Dieter; Daily, William; Ho, Samuel Klin Sangi; Frackman, Susan; Hawkins, Erika; Wood, Keith V.

PATENT ASSIGNEE(S): Promega Corporation, USA

SOURCE: PCT Int. Appl., 130 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2004027378 | A2 | 20040401 | WO 2003-US29078 | 20030916 |
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| CA 2497560 | A1 | 20040401 | CA 2003-2497560 | 20030916 |
| AU 2003267245 | A1 | 20040408 | AU 2003-267245 | 20030916 |
| AU 2003267245 | B2 | 20070712 | | |
| EP 1546162 | A2 | 20050629 | EP 2003-749715 | 20030916 |
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| JP 2006508339 | T | 20060309 | JP 2004-537859 | 20030916 |
| US 2004171099 | A1 | 20040902 | US 2003-665314 | 20030919 |
| PRIORITY APPLN. INFO.: | | | US 2002-412254P | P 20020920 |
| | | | US 2003-483309P | P 20030627 |
| | | | WO 2003-US29078 | W 20030916 |

OTHER SOURCE(S): MARPAT 140:299425

AB The present invention provides methods, compns., substrates, and kits useful for analyzing the metabolic activity in cells, tissue, and animals and for screening test compds. for their effect on cytochrome P 450 activity. In particular, one-step and two-step methods using luminogenic mol., e.g., luciferin or coelenterazines, that are cytochrome P 450 substrates and that are also bioluminescent enzyme, e.g., luciferase, pro-substrates are provided. Upon addition of the luciferin derivative or other luminogenic mol. into a P 450 reaction, the P 450 enzyme metabolizes the mol. into a bioluminescent enzyme substrate, e.g., luciferin and/or luciferin derivative metabolite, in a P 450 reaction. The resulting metabolite(s) serves as a substrate of the bioluminescent enzyme, e.g., luciferase, in a second light-generating reaction. Luminescent cytochrome P 450 assays with low background signals and high sensitivity are disclosed and isoform selectivity is demonstrated. The present invention also provides an improved method for performing luciferase reactions which employs added pyrophosphatase to remove inorg. pyrophosphate, a luciferase inhibitor which may be present in the reaction mixture as a contaminant or may be generated during the reaction. The

ACCESSION NUMBER: 2006:1279865 CAPLUS

DOCUMENT NUMBER: 146:57589

TITLE: Luminogenic and fluorogenic compounds and methods to detect molecules or conditions

INVENTOR(S): Daily, William; Hawkins, Erika; Klaubert, Dieter; Liu, Jianquani; Meisenheimer, Poncho; Scurria, Michael; Shultz, John W.; Unch, James; Wood, Keith V.; Zhou, Wenhui; Valley, Michael P.; Cali, James J.

PATENT ASSIGNEE(S): Promega Corporation, USA

SOURCE: PCT Int. Appl., 328pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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| WO 2006130551 | A2 | 20061207 | WO 2006-US20731 | 20060530 |
| WO 2006130551 | A8 | 20070201 | | |
| WO 2006130551 | A3 | 20070503 | | |
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| US 2007015790 | A1 | 20070118 | US 2006-444145 | 20060531 |
| PRIORITY APPLN. INFO.: | | | US 2005-685957B | P 20050531 |
| | | | US 2005-693034P | P 20050621 |
| | | | US 2005-692925P | P 20050622 |
| | | | US 2006-79045P | P 20060407 |

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
present method further provides a method for stabilizing and prolonging the luminescent signal in a luciferase-based assay using luciferase stabilizing agents such as reversible luciferase inhibitors.

IT 676460-20-1

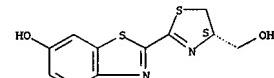
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-cyanobenzothiazole derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs., and pyrophosphatase, and drug screening applications)

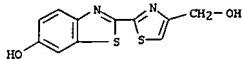
RN 676460-20-1 CAPLUS

CN 6-Benzothiazolol, 2-[{(4S)-4,5-dihydro-4-(hydroxymethyl)-2-thiazolyl}- (CA INDEX NAME)

Absolute stereochemistry.

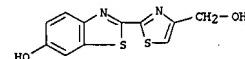


L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1997:763556 CAPLUS
 DOCUMENT NUMBER: 128:9275
 TITLE: Structure of the catalytic site of firefly luciferase and bioluminescence color
 AUTHOR(S): Brovko, L. Yu.; Dementieva, E. I.; Ugarova, N. N.
 CORPORATE SOURCE: Dep. Chem., Lomonosov Moscow State Univ., Moscow, 119899, Russia
 SOURCE: Bioluminescence and Chemiluminescence: Molecular Reporting with Photons, Proceedings of the International Symposium on Bioluminescence and Chemiluminescence, 9th, Woods Hole, Mass., Oct. 4-8, 1996 (1997), Meeting Date 1996, 206-211. Editor(s): Hastings, J. W.; Kricka, L. J.; Stanley, P. E. Wiley, Chichester, UK.
 CODEN: 65JYAO
 DOCUMENT TYPE: Conference
 LANGUAGE: English
 AB Time-resolved fluorescence was used to examine the dynamic behavior of active site Trp in luciferase from *Photinus pyralis* and *Luciola mingrellica*. *P. pyralis* luciferase exhibited a more rigid protein structure consistent with its higher thermostability. Fluorescence spectra of luciferin (phenolate form) and dehydroluciferin in different organic solvents together with the spectral characteristics of native bioluminescence and protein structure were analyzed to establish a correlation between active site microenvironment and bioluminescence color. The authors conclude that bioluminescence color is determined by both active site polarizability of the active site. The ability of nearby residues to rearrange around the emitter is also an important factor.
 IT 43094-08-2, Dehydroluciferol
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (correlation of firefly luciferase active site flexibility and polarizability and bioluminescence color)
 RN 43094-08-2 CAPLUS
 CN 6-Benzothiazolol, 2-[4-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)

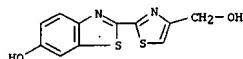


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1979:519909 CAPLUS
 DOCUMENT NUMBER: 91:119909
 TITLE: Synthesis of firefly luciferin and structural analogs
 AUTHOR(S): Bowie, Lemuel J.
 CORPORATE SOURCE: Lab. Serv., VA Hosp., San Diego, CA, 92161, USA
 SOURCE: Methods in Enzymology (1978), 57(Biolumin. Chemilumin.), 15-28
 CODEN: MENCHAU; ISSN: 0076-6879
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The synthesis of luciferin and analogs is described using the synthetic approach of S. Seto et al. (1963) for mechanistic studies of firefly luciferase. The procedure involves the reaction of carbamoylthiocarbonylthioacetic acid with p-anisidine to form 4-methoxythiocarboxanilamide which is cyclized to form 2-carbamoyl-6-methoxybenzothiazole. This is converted to the corresponding nitrile, and this is condensed with cysteine.
 IT 43094-08-2P
 RL: PREP (Preparation)
 (preparation of, for luciferase mechanistic studies)
 RN 43094-08-2 CAPLUS
 CN 6-Benzothiazolol, 2-[4-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1973:401911 CAPLUS
 DOCUMENT NUMBER: 79:1911
 TITLE: Synthesis of a new substrate analog of firefly luciferin. Active-site probe
 AUTHOR(S): Bowie, Lemuel J.; Horak, Vaclav; DeLuca, Marlene
 CORPORATE SOURCE: Sch. Med., Georgetown Univ., Washington, DC, USA
 SOURCE: Biochemistry (1973), 12(10), 1845-52
 CODEN: BICHAW; ISSN: 0006-2960
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB A new substrate analog of firefly luciferin was synthesized. The compound, 2-(6-hydroxy-2-benzothiazolyl)-4-hydroxymethylthiazole, (I) is an analog of dehydroluciferin, a competitive inhibitor of firefly luciferase. The spectral and enzymic properties of this analog suggest that it should be an ideal active-site for firefly luciferase.
 IT 43094-08-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 43094-08-2 CAPLUS
 CN 6-Benzothiazolol, 2-[4-(hydroxymethyl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



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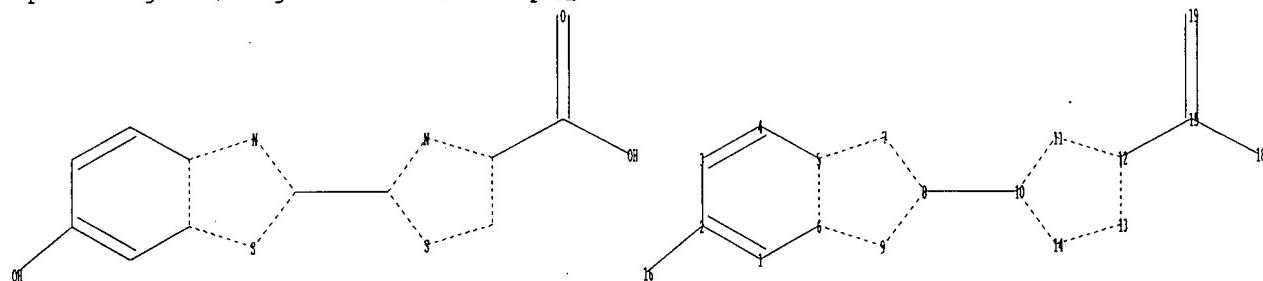
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<http://www.cas.org/support/stngen/stndoc/properties.html>

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ring bonds :
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13-14
  
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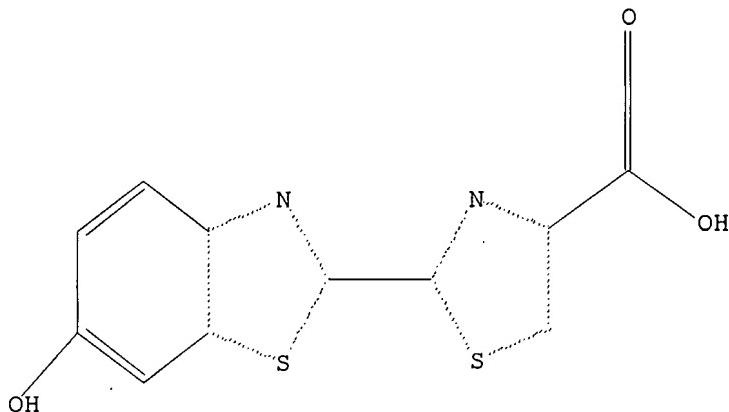
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G1:Cb,Cy,Hy,Ak

Match level :
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11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 18:CLASS 19:CLASS

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L5 STR



G1 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

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BATCH **COMPLETE**
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| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
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FILE COVERS 1907 - 5 Oct 2007 VOL 147 ISS 16
FILE LAST UPDATED: 4 Oct 2007 (20071004/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

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=> s 17
L8 865 L7

=> fil reg
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.47 | 371.70 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4
DICTIONARY FILE UPDATES: 4 OCT 2007 HIGHEST RN 949197-90-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

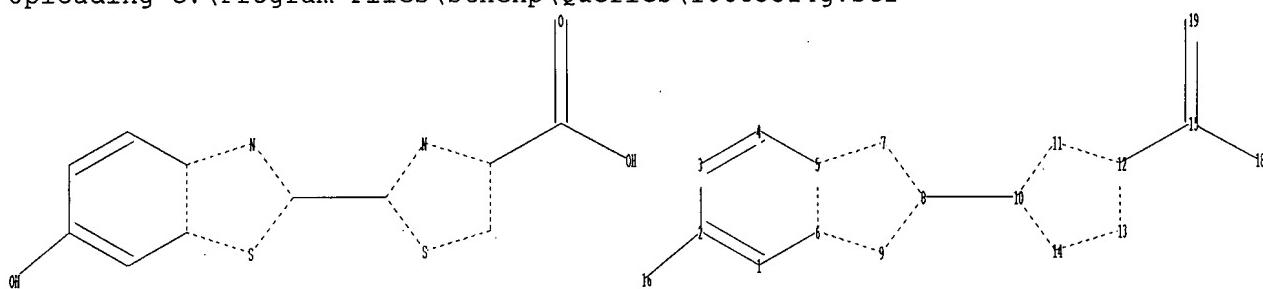
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10665314g.str



chain nodes :

15 16 18 19

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

2-16 8-10 12-15 15-18 15-19

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

exact/norm bonds :

2-16 5-6 5-7 6-9 7-8 8-9 10-11 10-14 11-12 12-13 13-14

exact bonds :

1-2 1-6 2-3 3-4 4-5 8-10 12-15

normalized bonds :

15-18 15-19

isolated ring systems :

containing 1 : 10 :

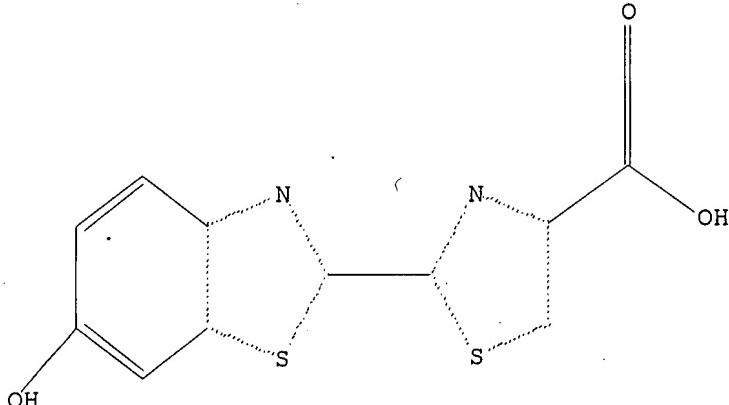
G1:Cb,Cy,Hy,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 18:CLASS 19:CLASS

L9 STRUCTURE UPLOADED

=> d
L9 HAS NO ANSWERS
L9 STR



G1 Cb,Cy,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 19
SAMPLE SEARCH INITIATED 14:23:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 189 TO ITERATE

100.0% PROCESSED 189 ITERATIONS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2956 TO 4604
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=> s 19 full
FULL SEARCH INITIATED 14:23:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4492 TO ITERATE

100.0% PROCESSED 4492 ITERATIONS
SEARCH TIME: 00.00.01

L11 0 SEA SSS FUL L9

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 172.10 543.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE 0.00 -3.90

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=> s 18 and luciferin
2841 LUCIFERIN
286 LUCIFERINS
2911 LUCIFERIN
(LUCIFERIN OR LUCIFERINS)
L12 823 L8 AND LUCIFERIN

| | | | |
|--|------------------|---------------|--|
| => log y | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 2.48 | 546.28 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -3.90 | |

STN INTERNATIONAL LOGOFF AT 14:24:21 ON 05 OCT 2007